

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -104 °C

Global applicability domain: Outside

Local applicability domain index: 5.99e-01

Confidence level: 7.58e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Perflenapent</div> <div>Measured: -100</div> <div>Predicted: -104</div>	<div>Image not found</div> <div>Perflexane</div> <div>Measured: -87.1</div> <div>Predicted: -99.4</div>	<div>Image not found</div> <div>Perfluorobutane</div> <div>Measured: -128</div> <div>Predicted: -125</div>
<div>Image not found</div> <div>Perfluoroisohexane</div> <div>Measured: -119</div> <div>Predicted: -109</div>	<div>Image not found</div> <div>1,1,1,2,2,3,4,4,5,5,5-Undecafluoro-3-(trifluoromethyl)pentane</div> <div>Measured: -115</div> <div>Predicted: -108</div>	